AMENDMENTS TO THE CLAIMS

1-2. (CANCELLED)

3. (CURRENTLY AMENDED) A computer-implemented method of constructing a model for predicting molecular behavior using marker molecules, said method comprising:

~~receiving data related to one or more chemical or biological properties of a set of reference molecules;~~

~~using said data,~~ classifying ~~the~~ respective molecules in ~~said~~ a set of reference molecules as either possessing or not possessing at least one chemical or biological property;

selecting a subset of said set of reference molecules, wherein all of the molecules in said subset possess the at least one property;

comparing all molecules in said set with all other molecules in said set in accordance with a pre-defined numerical similarity metric;

selecting a ~~first~~ target molecule ~~of~~ from said subset;

~~sorting all other molecules of said set in descending order of numerical similarity to said first molecule, thereby defining a similarity distance in terms of number of molecules between said first molecule and each other molecule of the set;~~

defining, for each ~~range in~~ other molecules ~~of similarity distance away from said first molecule~~in said set, a fractions-correctly-predicted metric as the number of molecules ~~in said range which are also members of said subset~~in said set that are members of said subset and that have a numerical similarity to said target molecule at least as great as said each other molecule's numerical similarity to said a target molecule divided by the total number of molecules ~~in said range~~in said set having a numerical similarity to said target molecule at least as great as said each other molecule's numerical similarity to said target molecule;

determining, from molecules in said set having a fractions-correctly-predicted metric below a threshold value, which molecule has the highest numerical similarity to said target molecule;

counting the number of molecules ~~away from said first molecule at which the fractions-correctly-predicted metric for said first molecule drops below a threshold~~

~~value~~in said set having a higher numerical similarity to said target molecule than said molecule determined in said determining step;

choosing said ~~first~~ target molecule as a marker molecule if said ~~first molecule has a fractions correctly predicted metric which exceeds said threshold value for a pre-selected minimum distance.~~number of molecules is equal to or greater than a pre-selected value.

4. (ORIGINAL) The method of Claim 3, wherein said subset comprises all of the molecules in said set that possess said at least one property.

5. (CANCELED)

6. (CURRENTLY AMENDED) The method of Claim 3, additionally comprising repeating said ~~counting~~ determining and counting steps for a plurality of different threshold values.

7. (CURRENTLY AMENDED) The method of Claim 3, comprising repeating said selecting a ~~first~~ target molecule, ~~sorting,~~ defining, determining, counting, and choosing steps for other molecules of said subset at a plurality of different threshold values and ~~minimum distances~~pre-selected number of molecules value so as to select a plurality of preliminary sets of marker molecules.

8. (ORIGINAL) The method of Claim 7, comprising choosing a final set of marker molecules by making molecular behavior predictions for all molecules in said set using each one of said preliminary sets of marker molecules, and choosing as said final set of marker molecules the preliminary set that most accurately predicts molecular behavior of molecules of said set.

9-18. (CANCELED)